

FUNDAMENTALS OF MOLD FREE CASTING: EXPERIMENTAL AND COMPUTATIONAL STUDIES

Prof. Gretar Tryggvason (P.I.)
 Prof. Steven Ceccio (co-P.I.)
 Mechanical Engineering and Applied Mechanics
 University of Michigan, Ann Arbor, MI 48109-2121
 (313)-764-4254
 (313)-764-4256 (FAX)
 gretar@engin.umich.edu
 ceccio@engin.umich.edu

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Objective

Researchers are developing the technology of "Ballistic Particle Manufacturing" (BPM) in which individual drops are precisely layered onto a substrate, and the drops are deposited so as to prevent splatting. These individual drops will ultimately be combined to form a net-shape, three-dimensional object. Our understanding of controlled drop deposition as applied to BPM is far from complete. Process parameters include the size and temperature of the liquid metal drop, its impact velocity and trajectory, and the condition and temperature of the substrate. Quantitative knowledge of the fluid mechanics and heat transfer of drop deposition and solidification are necessary to fully optimize the manufacturing process and to control the material microstructure of the final part. The object of this study is to examine the dynamics of liquid metal drops as they impinge upon a solid surface and solidify under conditions consistent with BPM (*i.e.* conditions which produce non-splating drops). A program of both numerical simulations and experiments will be conducted. Questions this study will address include the following:

- How do the deformation and solidification of the drop depend on the properties of the fluid drop and the solid substrate?
- How does the presence of previously deposited drops affect the impingement and solidification process? How does the impingement of the new drop affect already deposited material?
- How does the cooling rate and solidification of the drops influence the material microstructure?

Numerical Examination of Drop Deposition and Solidification

We use a unified approach to deal with fluid flow, heat transfer, and phase change during complex solidification processes. A single set of equations governing the conservation of mass, energy, and momentum are written for all phases involved and the phase boundary is treated as an imbedded interface by adding the appropriate source terms to the conservation laws. These source terms are in the form of delta functions localized at the interface and are selected in such a way to satisfy the correct matching conditions at the phase boundary. The resulting "one-field" Navier-Stokes equations are [1]:

$$\frac{\partial \rho \bar{u}}{\partial t} + \nabla \cdot \rho \bar{u} \bar{u} = -\nabla p + \bar{f} + \nabla \cdot \mu (\nabla \bar{u} + \nabla \bar{u}^T) + \int_F \bar{F}_s \delta(\bar{x} - \bar{x}_f) d\bar{a}$$

Here, \bar{u} is the velocity vector, p the pressure, and ρ and μ are the discontinuous density and viscosity fields, respectively. \bar{f} is a body force that can be used to initiate the motion. The surface forces, \bar{F}_s , act only on the interface between the different fluids and appears in the current formulation multiplied by a three-dimensional delta function, δ . The integral is over the entire front. It is important to note that this equation contain no approximations beyond those in the usual Navier-Stokes equations. In particular, it contains implicitly the proper stress conditions for the

fluid interface. The momentum equation is supplemented by an equation of mass conservation. For incompressible flows this leads to an elliptic equation for the pressure. To advect the material properties, and to evaluate the surface tension term in the momentum equation, we track the interface between the different phases explicitly by using a moving grid of lower dimension than what we use for the conservation equations. This grid is usually referred to as a front. The one-field formulation used here is common to other techniques for multifluid flows such as the VOF (Volume of Fluid) and level set methods. In these methods, however, the phase boundary is not tracked explicitly, but reconstructed from a marker function. Explicitly tracking the interface avoids the difficulty of advecting such marker function and allows accurate evaluation of surface forces. This formulations has been used to examine the dynamics of fluid drops and bubbles in the following work: [2, 3, 4, 5].

The approach taken for the fluid flow, works also for heat flow and phase changes. In Juric and Tryggvason [6] we developed a method to simulate phase changes in a pure material in the absence of any fluid motion. With these assumptions we have only to solve one heat conduction equation:

$$\frac{\partial \rho c T}{\partial t} = \nabla \cdot k \nabla T + \int_F \dot{q} \delta(\bar{x} - \bar{x}_F) da$$

where \dot{q} is adjusted in such a way that the temperature of the interface is given by the Gibbs-Tompson conditions

$$T_F = T_M \left(1 - \frac{\sigma \kappa}{L} \right)$$

Here, T_M is the melt temperature, T_F is the temperature at the front, κ is the conductivity, and L is the volumetric latent heat. Additional terms can be added to the right hand side to account for variability in surface tension as well as anisotropy. We have compared the method with exact solutions for stable solidification and found excellent agreement, even with relatively coarse resolution. The same approach can also be used for the solidification of binary alloys where the solidification temperature depends on the composition of the melt. In this case we also need to solve an equation for the solute concentration [7, 8]. For real multiphase flows, the fluid code and the phase change have to be combined. This introduces additional complications, such as a volume source at the phase boundary, that can be dealt with in several ways.

Numerical Results

The method described above has been used to simulate the pure and binary solidification of non-flowing systems [9]. These simulations have captured interfacial instabilities during solidification and the growth of dendritic structures. Although predicting the microstructure formation during solidification is a problem of immense importance and complexity (and we have only addressed relatively simple aspect so far), it is one aspect of predicting the solidification of a realistic system. Often, the range of scales between the size of the microstructures and the dimensions of the system we need to predict are very large and resolving the formation of every microstructure is completely impractical. In those cases it is necessary to make some assumptions about what happens at the small scale level in order to be able to resolve the large scale features of the system. How the collective behavior of small scale features is manifested at larger scales is, of course, a central problem in the modeling of physical system and is far from a solved problem. In fluid/solidification simulations some success has been achieved by allowing for a "mushy zone" at the boundary between a fluid and a solid which represents a partially solidified region consisting of fluid and microstructures such as dendrites. We have simulated drops colliding with cold walls with an even simpler model where we simply assume that a melt solidifies if its temperature falls below the solidification temperature. Although simple, this model captures at least some aspects of the interaction of fluid flow and solidification. Figure 1 shows the collision and solidification of two drops at three times. In the first frame the first drop has already collided with the wall and is

partially solidified. In the second frame the first drop is completely solid but the second drop is still fluid. In the third frame both drops have solidified. In this simulation the drop Weber number is high so the drops deform greatly and the drop thermal conductivity is low so the drops have time to deform before they solidify. In figure 2, however, where we show two drops after they have solidified the conductivity is high and Weber number low, thus resulting in much less deformations. In these simulations we solve for the motion of both the fluid in the drop as well as the ambient fluid. Figure 3 shows the temperature in both the drop and the fluid as well as the streamlines at a time when the first drop has solidified but the second has not. We see that the bottom drop has reached the temperature of the wall, but the second still has essentially its original temperature. Since the drop loses heat to the ambient fluid, a thermal wave is clearly visible.

Experimental Examination of Drop Deposition and Solidification

The experimental examination of drop deposition and solidification required the construction of an apparatus which can controllably create a single drop of prescribed size which will then be propelled toward a sub-cooled substrate. A drop ejector has been devised to create and deliver a drop of liquid material. The drop must be uniformly melted and the velocity and trajectory of the drop must be repeatable. Once ejected, the drops will travel to the substrate. The substrate is mounted on a computer controlled X-Y traverse, and a substrate can be moved to provide a virgin surface for drop deposition or move a previously deposited drop into the impact zone of an incoming drop. The table has been constructed to accommodate a variety of different substrate materials. The experiments will be conducted in a vacuum chamber to eliminate the effect of an ambient atmosphere on the drop deposition process. A variety of instrumentation will be used to quantitatively monitor the deposition process such as still and motion image acquisition, dynamic temperature acquisition, and IR imaging. We have used Gallium, Wood's metal, and Rose's metal as materials in our preliminary experiments. Images of the deforming and solidifying drops acquired to date are qualitatively similar to the numerical predictions.

Need For Experiments in Microgravity

Experimental studies of drop deposition can be significantly enhanced if performed in microgravity. In terrestrial applications of BPM, small drops are used and gravity is important. However, it is quite difficult to quantitatively observe small, fast moving drops, and thus we would like to scale up the size of the drops. This leads to the well known difficulty that while gravity may be negligible for the small drop, it is likely to be the dominant effect for a drop that is sufficiently large to be easily observable. A microgravity environment would permit the proper scaling of the experiment. For high Reynolds numbers both experiments and numerical simulations show that the drop deformation is only weakly dependent on the Reynolds number. Thus, in the absence of gravity, the drops can be made larger for a given Weber number simply by reducing their velocity. Dimensionless parameters associated with the process of heat transfer and solidification of the drop are the Prandtl and Stefan numbers which would not be effected by a change of size scale. The time constants associated with these processes are proportional to the square of the drop diameter for given thermal conductivities of the liquid drop and substrate material and given temperature differences. By scaling up the drop size it also becomes easier to observe the slower process of drop heat exchange and solidification. Consequently, the microgravity environment offers unique opportunities to study the complete process of drop deposition and solidification in detail by examining large, slowly moving drops.

Significant Results to Date

We have used a pilot grant from NASA to initiate our research effort. Significant Results are summarized below:

- We have developed the capability to simulate the deformation of multiple metal drops as they impinge on a substrate. These are fully resolved, three-dimensional calculations.
- These simulations have been extended to include the solidification of drops of pure material, and we expect that these simulations can be extended to binary solutions.
- We have developed a drop producing apparatus which is capable of producing individual drops of liquid metal. We are modifying this device to ensure its function in a microgravity environment.
- The traverse and cooling system for the substrate has been developed, and a design of the vacuum chamber has been completed.

We have conducted experiments in which relatively large metal drops are dropped into hot oil which will impinge and solidify on a cooled substrate. data from these is being compared with numerical simulations. The role of direct numerical simulations in material processing is currently in its infancy, but the prospect that it will ultimately have a significant impact are enormous. Several groups are currently active in various aspects of such simulations. We have presented a unified approach for heat transfer, phase changes and fluid flow that is applicable both for exploration of the formation of small scale structures as well as to more global aspects of the solidification process where the details of the microstructure are not resolved.

Acknowledgments

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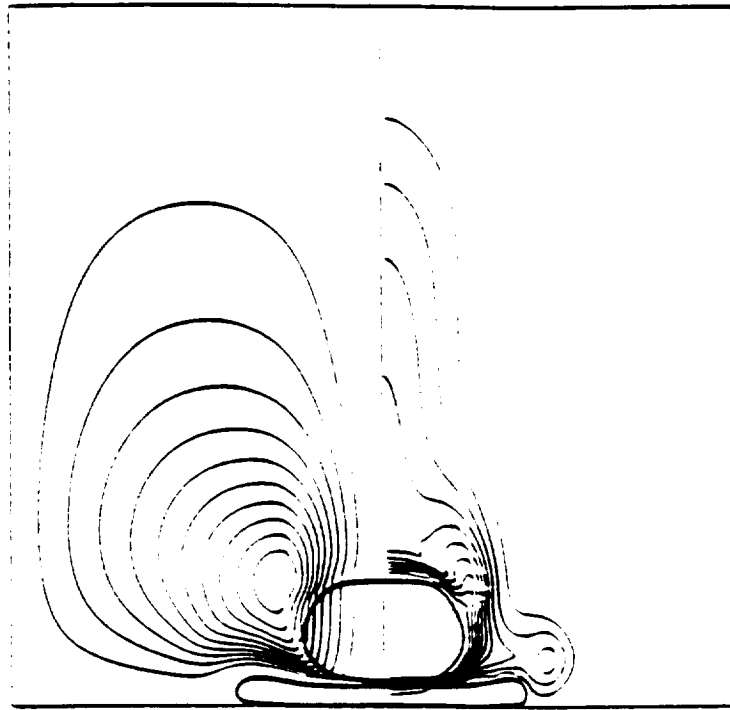


Figure 2. The temperature field and the streamlines for the drops in Figure 3 as the first drop has collided with the wall and solidified and the second drop is just about to collide with the first one. Since both the flow in the drops as well as the ambient fluid are simulated, we plot the contour values there also. Here, no streamlines cross the bottom drop, indicating that it is fully solidified. A large thermal wave is left behind the drops and hot wake fluid is entrained in a vortex formed by the wake fluid that is moving outward near the bottom.

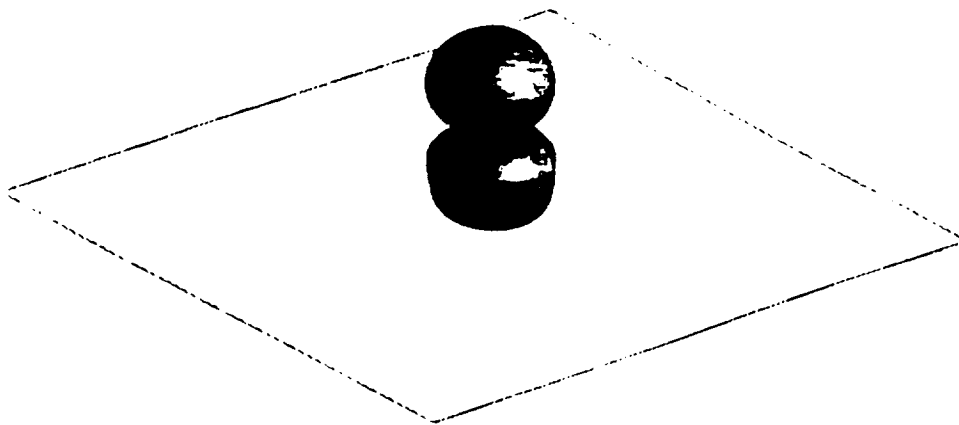


Figure 3. The final, solidified shape of two drops colliding with a cold wall. In this case the Weber number is low and thermal conductivity high, so the drops do not deform much and solidify rapidly as they hit the wall.

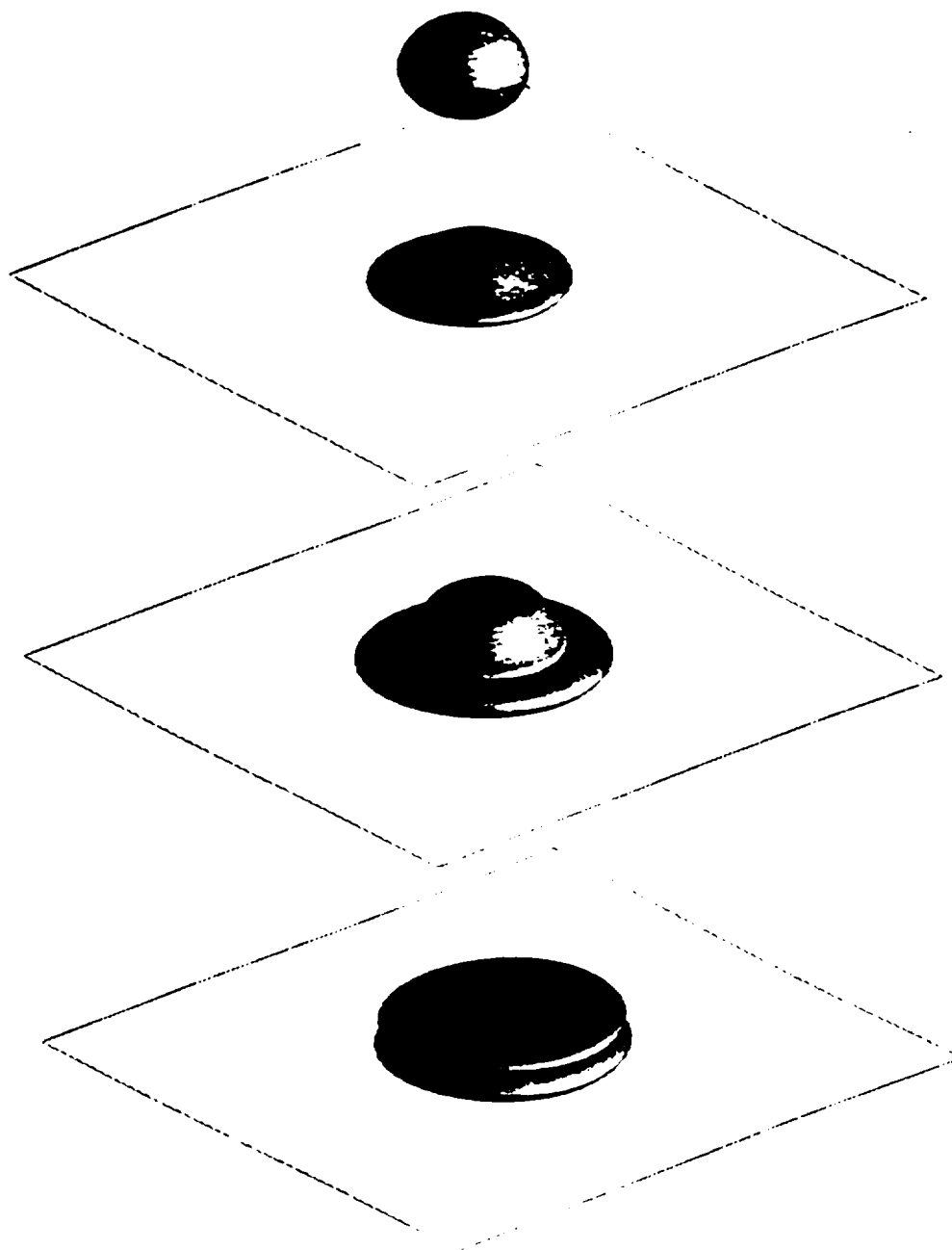


Figure 1. The solidification of a two drops colliding with a cold wall. In the top frame the first drop is splatting on the wall, but has not solidified yet. In the middle frame the first drop has completely solidified, but the second drop has not. Both drops have solidified in the bottom frame. In this case the drops are not allowed to coalesce. The thermal conductivity is relatively low and the Weber number high, thus resulting in highly deformed drops after solidification.